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# Stability for implicit–explicit schemes for non-equilibrium kinetic systems in weighted spaces with symmetrization ☆

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ABSTRACT

We consider kinetic systems, and prove their stability working in weighted spaces in which the systems are symmetric. We prove stability for various explicit and implicit semi-discrete and fully discrete schemes. The applications include advective and diffusive transport coupled to the accumulation of immobile components governed by non-equilibrium relationships. We also discuss extensions to nonlinear relationships and multiple species.



## 1. Introduction

In this paper we transform and analyze semi-implicit numerical schemes for an evolution system

$$(\phi u)_t + v_t + \nabla \cdot (qu) - \nabla \cdot (\phi d \nabla u) = f, \tag{1a}$$

$$v_t = \alpha(g(u) - v) \tag{1b}$$

which arises in a variety of important applications, e.g., transport in porous media with adsorption. Here $\alpha > 0$ and $g(\cdot)$ is monotone, with details below. The positive coefficient $\phi$ is the porosity.

For this system there is no maximum principle, and if $f = 0$, there is not even a natural conservation or stability principle in the natural norms of $(u, v)$. Further, the analysis of the simple finite discretization schemes with well known truncation errors, even when $g$ is linear, has to deal with nonnormality, and is unnecessarily complex, even when $g(\cdot)$ is linear.

The transformation we propose involves symmetrization, rescaling, and a change of variables. Equivalently, we work in weighted spaces. We exploit the symmetrization to prove strong stability of the problem and of the associated numerical schemes, from which the natural error estimates follow. For fully implicit schemes the framework of m-accretive operators reduces the stability analysis to the verification that the operator is m-accretive. However, for implicit–explicit schemes this is not sufficient, and we draw upon Fourier analysis.

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*Overview.*

For the linear case when $g(u) = cu$, with $c > 0$, the abstract form of (1) has the structure of a linear kinetic system

$$U' + V' + LU = F \tag{2a}$$

$$V' + \alpha(V - cU) = 0, \tag{2b}$$

with the unknowns $U, V : (0, T] \rightarrow H \times H$, where $H$ is an appropriate Hilbert space to be defined, and the source term $F : [0, \infty) \in H$ is given. The linear transport operator $L$ is defined in the sequel, and we will require for $L$ to be m-accretive to get strong stability.

Our main technical objective is to study the stability of (2) and of one-step implicit and implicit–explicit discrete schemes for (2)

$$\frac{U^n - U^{n-1}}{\tau} + \frac{V^n - V^{n-1}}{\tau} + LU^{n*} = F^n \tag{3a}$$

$$\frac{V^n - V^{n-1}}{\tau} + \alpha(V^n - cU^n) = 0, \tag{3b}$$

which is solved at every time step $n = 1, 2, \ldots$ for the approximations $U^n, V^n$ to $u(\cdot, t_n), v(\cdot, t_n)$. Here $F^n \approx F(t_n)$. This one-step scheme is fully implicit if $n* = n$. Other schemes arise for $n* \neq n$. The analysis of (3) involves consideration of spatial discretization as well as of time discretization. Our technique of symmetrization allows to demonstrate strong stability of the schemes in a weighted space, even though the original system (2) has nonnormal operators.

Extensions of (2) to nonlinear systems and to systems with multiple components will be also discussed.

*Motivation and context.*

The problem (1) comes from applications in subsurface modeling such as the transport of contaminant undergoing adsorption, or coalbed methane reservoir simulation, but cover also a variety of other applications. In those problems (1) represents the conservation of mass of some chemical component, with $u$ denoting the mobile concentration, and $v$ representing the immobile component, while $g(\cdot)$ a general monotone (increasing) function. We provide details on the applications in Section 2.

Numerical analysis of (1) with non-equilibrium kinetics was given in [1] for diffusion only, with focus on non-Lipschitz $g(\cdot)$ important for liquid adsorption. In [2] Lagrangian techniques for advection with non-equilibrium adsorption and in [3] the Lagrangian transport combined with Galerkin approximation to diffusion were analyzed. In addition, in a sequence of papers devoted to the scalar conservation laws with relaxation terms [4] a problem similar to (4a) but without diffusion is studied, and convergence order of $O(\sqrt{h})$ is established. In turn, in [5] we studied the stability of schemes for a single equation analogue of (4a) without diffusion and where $v$ was eliminated, and in [6] we extended the analysis to cover the linear case with diffusion. Furthermore, previous results on stability of schemes of (2) for the case of initial equilibrium were shown in [5–7].

Our approach in this paper provides a unified framework for the analysis of a variety of explicit and implicit finite difference schemes for the non-equilibrium advection–diffusion problems. In particular, it establishes strong stability as well as optimal error estimates of order $O(h)$ or $O(h^2)$.

*Outline.*

In Section 2 we motivate the study of (2), provide examples of $L$, and provide literature review. In Section 3 we describe the main idea of symmetrization in the abstract setting leading to the stability of the numerical schemes. In Section 4 we provide concrete examples of fully discrete schemes for (2) and evaluate their stability, and in Section 5 we illustrate the theory with numerical examples, and convergence studies. We close in Section 6, where we outline extensions to the nonlinear and multi-species case, and discuss future work.

*Notation and assumptions.*

Throughout the paper we assume that $c > 0$, $\alpha > 0$; otherwise, the system is decoupled and trivial. $I$ always denotes the identity operator or matrix, as is clear from the content.

With the original variables in (1) denoted by $u(x, t)$ and $v(x, t)$, we consider the vectors $U(t) = u(\cdot, t) = (u(x, t))_x \in H$. Each $U(t), V(t)$ lives in a Hilbert space $H$, with the inner product denoted by $\langle \cdot, \cdot \rangle_H$; we drop the subscript $H$ when it does not lead to a confusion. The domain of an operator $L$ is denoted by $D(L)$, and the time derivative $U'(t)$ or $\frac{dU}{dt}(t)$ generalizes the partial derivative $\frac{\partial}{\partial t}$, and is defined in an appropriate abstract setting, such as that developed in [8].

The vector $W = W(t) = [U(t), V(t)]^T$ lives in $H \times H$, which is endowed either with the natural or weighted inner product, with details below. We also consider new variables $\tilde{W}$ in appropriate spaces. The (matrices of) operators on $W$ or $\tilde{W}$ in the